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A COMPARISON OF THE EXISTENCE THEOREMS OF KANTOROVICH AND MOORE--ETC(U)
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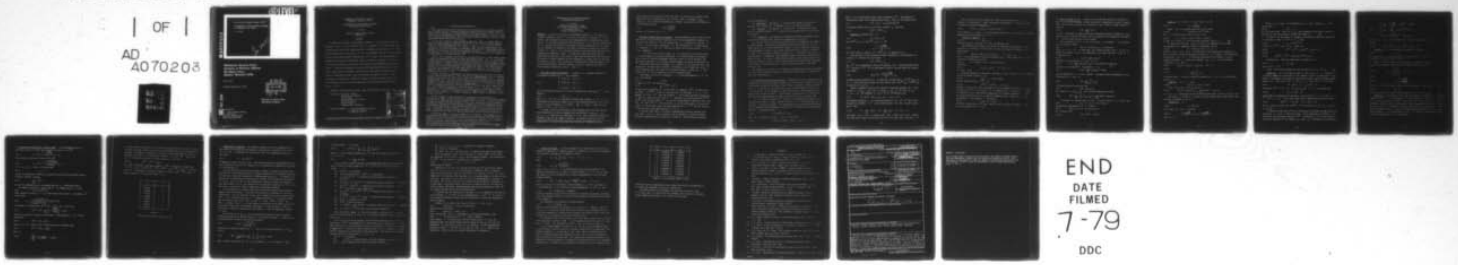

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A COMPARISON OF THE EXISTENCE THEOREMS OF KANTOROVICH AND MOORE

L. B. Rall

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ABSTRACT

In order to be useful, an approximate solution y of a nonlinear system of equations $f(x) = 0$ in R^n must be close to a solution x^* of the system. Two theorems which can be used computationally to establish the existence of x^* and obtain bounds for the error vector $y - x^*$ are the 1948 result of L. V. Kantorovich and the 1977 interval analytic theorem due to R. E. Moore. The two theorems are compared on the basis of sensitivity (ability to detect a solution x^* close to y), precision (ability to give sharp error bounds), and computational complexity (cost). A theoretical comparison shows that the Kantorovich theorem has at best only a slight edge in sensitivity and precision, while Moore's theorem requires far less computation to apply, and thus provides the method of choice. This conclusion is supported by a numerical example, for which available UNIVAC 1108/1110 software is used to check the hypotheses of both theorems automatically, given y and f.

AMS(MOS) Subject Classifications: 65H10, 65G99 (Interval analysis), 68A20

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Significance and Explanation

This report shows a way to save money in the evaluation of accuracy of approximate solutions of finite systems of nonlinear algebraic and trancendental equations, based on the comparison of an older method for this purpose with a newer one. It is shown that the two methods are theoretically about equally effective, while the newer one is cheaper computationally. This conclusion has been verified in practice, using operational UNIVAC 1108/1110 software.

In the case of finite linear systems of equations, there is a simple theory based on a finite number of arithmetic operations. For linear systems of moderate size, the successful computation of a vector $y = (y_1, y_2, \ldots, y_n)$ can imply that it is close to the actual solution $x^* = (x_1^*, x_2^*, \ldots, x_n^*)$. For nonlinear systems, the situation is less well understood in both theory and practice, although many numerical methods are known which will furnish approximate solutions y. The concern here is not with how y has been found, but rather with the determination of its accuracy as an approximation to an exact solution x^*.

Often, x^* is defined as the limit of an infinite process, so the computed value y will be contaminated by both truncation and roundoff error. For y to be useful, one must be able to assert that it is satisfactorily close to x^*. In order of increasing expense, such assertions can be based on simple (but perhaps misguided) faith in the output of a computer, usually reliable but not truly rigorous heuristic observations, or the use of theorems which give guaranteed results. The latter degree of certainty may be required in certain applications, in addition to its intellectual necessity, and involves proving the <u>existence</u> of x^* as well as obtaining <u>error bounds</u> for the vector $y - x^*$.

Certain criteria are established for theorems which prove existence of solution vectors and give error bounds. First, they must be <u>computational</u>, so that a computer program can be written to check out the hypotheses of the theorem, given y and the system of equations. Thus, the proof of existence and error bounds will be provided automatically, or an indication of the reason for failure of the theorem to hold will be given. A second desirable property is <u>sensitivity</u>; if y is close to a solution, then the theorem should detect the existence of x^* rather than give a negative result. Also wanted is <u>precision</u>, so that the bounds for $y - x^*$ will be as sharp as possible, to help avoid wasting money by refining an already sufficiently accurate approximation. Finally, the theorem should be as <u>simple</u> (cheap) to implement as possible. The computation of y might be expensive, and as little as necessary should be added to this.

A metric existence theorem suitable for automation was published by L. V. Kantorovich in 1948. At MRC, software for implementation of this theorem was announced in 1967, and an improved version was released in 1972. In 1977, R. E. Moore published an interval analytic existence theorem to which this software was readily adaptable, as automatic differentiation and interval arithmetic were already implemented in it. A theoretical comparison of these theorems of different type is achieved by recasting Moor 's theorem as a metric theorem. It turns out that the Kantorovich theorem has only a slight edge in sensitivity and precision over this restricted version of the Moore theorem, but the latter is computationally much simpler and hence preferable.

A numerical example is given to support this conclusion. This example arose in an unrelated investigation of numerical solution of nonlinear integral equations of radiative transfer type, and was not constructed for this purpose. The use of Moore's theorem gave a 4 to 1 advantage in speed, and detected the existence of a solution which the supposedly more sensitive Kantorovich theorem failed to do.

A COMPARISON OF THE EXISTENCE THEOREMS OF KANTOROVICH AND MOORE

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ABSTRACT. In order to be useful, an approximate solution y of a nonlinear system of equations $f(x) = 0$ in R^n must be close to a solution x^* of the system. Two theorems which can be used computationally to establish the existence of x^* and obtain bounds for the error vector $y - x^*$ are the 1948 result of L. V. Kantorovich and the 1977 interval analytic theorem due to R. E. Moore. The two theorems are compared on the basis of sensitivity (ability to detect a solution x^* close to y), precision (ability to give sharp error bounds), and computational complexity (cost). A theoretical comparison shows that the Kantorovich theorem has at best only a slight edge in sensitivity and precision, while Moore's theorem requires far less computation to apply, and thus provides the method of choice. This conclusion is supported by a numerical example, for which available UNIVAC 1108/1110 software is used to check the hypotheses of both theorems automatically, given y and f.

1. Nonlinear Systems of Equations. A system of n nonlinear algebraic or transcendental equations in n real unknowns,

$$(1.1)\qquad \begin{cases} f_1(x_1,x_2,\ldots,x_n) = 0 , \\ f_2(x_1,x_2,\ldots,x_n) = 0 , \\ \quad\ldots\quad\ldots\quad\ldots\quad\ldots \\ f_n(x_1,x_2,\ldots,x_n) = 0 , \end{cases}$$

may be represented concisely in the real n-dimensional vector space R^n as the equation

$$(1.2)\qquad f(x) = 0 ,$$

where $f: D \subset R^n \to R^n$ is a nonlinear operator from a domain $D \subset R^n$ into R^n. The problem of solving the system (1.1) or the equivalent equation (1.2) is, of course, to find a *solution* $x^* = (x_1^*,x_2^*,\ldots,x_n^*) \in D$ which f maps into the origin $0 = (0,0,\ldots,0)$ of R^n.

In order to keep the discussion of this problem within the realm of practical computation, it will be assumed that the functions $f_i(x_1,x_2,\ldots,x_n)$, $i = 1,2,\ldots,n$, comprising the components of $f(x)$ can be written as formulas in FORTRAN or some similar computer language. As software exists for analytic

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differentiation of functions of this type [4,9], it will also be assumed without further ado that the derivatives $f'_{ij} = \partial f_i/\partial x_j$ and, if necessary, $f''_{ijk} = \partial^2 f_i/\partial x_j \partial x_k$ can be computed automatically, so that, in particular, the evaluation of the Jacobian matrix

$$f'(x) = \left(\frac{\partial f_i(x)}{\partial x_j}\right) \tag{1.3}$$

presents no difficulty for $x \in D$.

2. Existence theorems and error bounds. Actual computation with one of the many methods for solving systems of equations will yield an *approximate solution* y , which will be useful if it can be asserted that y is "close" to a solution x^* of (1.2). This involves establishing (i) the *existence* of x^* in some region Ω^* containing y , and (ii) some type of *bound* for the *error vector* $\varepsilon = x^* - y$ or its components.

In the case of linear systems $Ax = b$, verification of existence rests on a finite number of aritimetic operations. For linear systems of reasonable size, errors in computed approximate solutions result only from rounding, and successful execution of a carefully written program can insure the existence of x^* and provide usable error estimates [2]. However, in the nonlinear case, such assurance of existence may be lacking. Furthermore, even if known to exist, x^* may be defined only as the limit of an infinite process, in which case y will differ from x^* due to truncation as well as roundoff error.

Some common criteria for accepting y as a good approximation to x^* are (i) the *residual*

$$r = f(y) \tag{2.1}$$

is small, or (ii) the *correction*

$$\delta_k = x^{(k+1)} - x^{(k)} \tag{2.2}$$

is small when calculating x^* as the limit of a sequence $\{x^{(k)}\}$, in which case one takes $y = x^{(k+1)}$. Either of these can fail for nonlinear f in R . For example, if $f(x) = e^{-x}$, then the residual r can be made arbitrarily small, but x^* does not exist such that $f(x^*) = 0$. Similarly, an iteration process $x^{(k+1)} = \phi(x^{(k)})$ can stall far from x^* . To see this, apply Newton's method to (1.2) with $f(x) = x^m$ and $x^{(0)} = 1$. The correction δ_0 can be made as small as desired by taking m sufficiently large; the value obtained for $y = x^{(1)}$ will be close to 1 and thus not a good approximation to $x^* = 0$.

It follows that there is a need for *computational* existence theorems such that given y and f , their hypotheses can be checked by a computer program, and error bounds obtained if existence is verified. Other desirable properties

for such theorems are:

(i) Sensitivity. The region Ω^* in which the theorem can detect the existence of a solution x^* of equation (1.2) is as large as possible.

(ii) Precision. The region Ω^* in which x^* is guaranteed to exist does not extend far beyond x^*, so that the error bounds obtained are as good as possible.

(iii) Simplicity. The additional computation required to guarantee existence and obtain error bounds should be as inexpensive as possible.

To a certain extent, sensitivity and precision are incompatible, at least in a single theorem. A sensitive theorem might establish existence of x^* in a large region, but not yield usable error bounds. A result requiring highly precise approximate solutions, on the other hand, might fail to detect a solution x^* which is close enough to make the accuracy of y satisfactory for the intended purpose. Consequently, some compromise between sensitivity and precision must be struck. Of course, a computational strategy can be devised in which a sensitive theorem is used to scout a large region for suitable initial approximations, which are then refined until a precise theorem guarantees sufficient accuracy [13].

The purpose of this paper is to compare two computational existence theorems, for which UNIVAC 1108/1110 software is operational, on the basis of sensitivity, precision, and simplicity.

3. The theorems of Kantorovich and Moore. Theorems which can be implemented computationally to obtain verifiable conditions for existence of solutions as well as error bounds include the well-known result on the convergence of Newton's method due to L. V. Kantorovich [6] and the more recent interval-analytic theorem of R. E. Moore [12]. Brief statements of these theorems will now be given; proofs may be found in the literature. In particular, a neat proof of the form of the Kantorovich theorem presented here may be found in the note by Ortega [14].

Let $\|\cdot\|$ denote a norm for R^n and also a consistent matrix norm for $n\times n$ real matrices; that is, $\|Ax\| \le \|A\|\cdot\|x\|$ for all $x \in R^n$ and square matrices A of order n with real elements. The ingredients of the Kantorovich theorem are (i) an *initial point* (approximate solution) $x^{(0)}$ at which the Jacobian matrix $f'(x^{(0)})$ is invertible, with

$$\|[f'(x^{(0)})]^{-1}\| \le B_0 , \tag{3.1}$$

and (ii) a Lipschitz constant κ for f' such that

$$\|f'(u) - f'(v)\| \le \kappa\|u-v\|, \quad u,v \in \Omega , \tag{3.2}$$

where Ω is a sufficiently large region containing $x^{(0)}$. (The meaning of "sufficiently large" will be made precise below.) From (i), the *Newton point*

$$x^{(1)} = x^{(0)} - [f'(x^{(0)})]^{-1} f(x^{(0)}) \tag{3.3}$$

is uniquely defined, and one can find a constant η_0 such that

$$\|x^{(1)} - x^{(0)}\| \leq \eta_0 . \tag{3.4}$$

Theorem 3.1 (Kantorovich). If

$$h_0 = B_0 \kappa \eta_0 \leq \frac{1}{2} , \tag{3.5}$$

and $\bar{U}(x^{(0)},\rho_0) = \{x : \|x-x^{(0)}\| \leq \rho_0\} \subset \Omega$ for

$$\rho_0 = \frac{1 - \sqrt{1-2h_0}}{h_0} \eta_0 , \tag{3.6}$$

then there exists a solution $x^* \in \bar{U}(x^{(0)},\rho_0)$ of equation (1.2).

The conclusion of this theorem provides a guarantee of the existence of a solution x^* and also the error bound

$$\|x^* - x^{(0)}\| \leq \rho_0 \tag{3.7}$$

for $x^{(0)}$ as an approximate solution of equation (1.2). Using the Newton point $x^{(1)}$ instead of $x^{(0)}$ as the approximate solution, one can obtain the sharper error bound

$$\|x^* - x^{(1)}\| \leq \frac{1-h_0 - \sqrt{1-2h_0}}{h_0} \eta_0 , \tag{3.8}$$

as shown by Gragg and Tapia [3]. In practice, one may take $\Omega = \bar{U}(x^{(0)},2\eta_0)$, as if κ is the Lipschitz constant for this region, then $\bar{U}(x^{(0)},\rho_0) \subset \bar{U}(x^{(0)},2\eta_0) = \Omega$ if and only if $h_0 \leq \frac{1}{2}$.

Moore's theorem is based on the concepts of interval analysis [11]. Given vectors $a = (a_1,a_2,\ldots,a_n)$ and $b = (b_1,b_2,\ldots,b_n)$ in R^n with $a_i \leq b_i$, $i = 1,2,\ldots,n$, the *interval* $X = [a,b]$ in R^n is defined to be

$$X = [a,b] = \{x : a_i \leq x_i \leq b_i,\ i = 1,2,\ldots,n\}. \tag{3.9}$$

The *interval extension* G of a continuous function $g:D \subset R^n \to R^n$ may be constructed on intervals $X \subset D$ in the following way: For $g(x) = (g_1(x), g_2(x),\ldots, g_n(x))$, take

$$c_i = \min_{u \in X} g_i(u) , \quad d_i = \max_{v \in X} g_i(v), \quad i = 1,2,\ldots,n , \tag{3.10}$$

and define $G(X) = [c,d]$. It follows that $G(X) \supset \{g(x) : x \in X\} = g(X)$; however, $G(X)$ may also contain vectors which are not of the form $g(x)$ for some $x \in X$.

The recipe for Moore's theorem [12] calls for an initial point y, an interval X containing y, and a nonsingular real matrix Y. These are used to form the *Krawczyk transformation*

$$K(X) = y - Yf(y) + \{I-YF'(X)\}(X-y) \tag{3.11}$$

of the interval X, where I is the identity matrix, and F' denotes the interval extension of the derivative f' of f.

Theorem 3.2 (Moore). If

$$K(x) \subset X , \tag{3.12}$$

then there exists a solution $x^* \in K(X)$ of equation (1.2).

This theorem also provides error bounds in addition to a guarantee of the existence of a solution. Setting $K(X) = [c,d]$, one obtains the componentwise error bounds

$$|x_i^*-y_i| \leq \max \{|y_i-c_i|,|d_i-y_i|\} , \quad i = 1,2,\ldots,n, \tag{3.13}$$

for y as an approximate solution of equation (1.2). Error bounds analogous to (3.8) may be obtained by setting

$$w = y-Yf(y), \quad [s,t] = \{I-YF'(X)\}(X-y) , \tag{3.14}$$

from which

$$|x_i-w_i| \leq t_i-s_i, \quad i = 1,2,\ldots,n, \tag{3.15}$$

as $(x-w) \in [s,t]$.

Although different in appearance, Theorems 3.1 and 3.2 have a common background. Define the *Newton operator* ϕ by

$$\phi(x) = x - [f'(x)]^{-1}f(x) , \tag{3.16}$$

and the *Newton sequence* $\{x^{(k)}\}$ by

$$x^{(k+1)} = \phi(x^{(k)}), \quad k = 0,1,2,\ldots . \tag{3.17}$$

Theorem 3.1 gives sufficient conditions for the convergence of the Newton sequence starting from $x^{(0)}$ to a solution x^* of equation (1.2). The Krawczyk operator K defined by (3.11) stems from an adaptation of the Newton operator (3.16) and the iteration process (3.17) to interval computation [8]. Under the hypotheses of Theorem 3.2, the operator ψ defined by

$$\psi(x) = x - Y f(x) \tag{3.18}$$

will have a fixed point $x^* \in K(X)$, which is also a solution of equation (1.2) by the invertibility of Y [12].

4. Moore's theorem in R^n_∞. Because of the different character of Theorems 3.1 and 3.2, it will be necessary to make some special assumptions in order to compare them. As the metric topology for intervals [11, pp. 15-24] is closely related to the norm

$$\|x\| = \max_{(i)} \{|x_i|\} \tag{4.1}$$

for R^n_∞, the method of comparison will be to reformulate Moore's theorem as a (less general) metric theorem, which will then be compared to the Kantorovich theorem in R^n_∞. The following concepts will be needed.

The closed ball $\bar{U}(y,\rho)$ in R^n_∞ with center y and radius ρ is a special type of interval, namely

$$\bar{U}(y,\rho) = \{x:\|x-y\| \leq \rho\} = [y-\rho e, y+\rho e] , \tag{4.2}$$

where $e = (1,1,\ldots,1)$. In particular, the *closed unit ball* $\bar{U}(0,1)$ in R^n_∞ is simply the interval $[-e,e]$. The *magnitude* of the scalar interval $[\alpha,\beta]$ in R is defined to be

$$|[\alpha,\beta]| = \max\{|\alpha|,|\beta|\} . \tag{4.3}$$

Similarly, for an interval $X = [a,b]$ in R^n,

$$|X| = \max_{(i)} \{\max(|a_i|,|b_i|)\} = \max\{\|a\|,\|b\|\} = \max_{x\in X} \|x\| \tag{4.4}$$

in terms of the norm (4.1). The *width* of X is

$$w(X) = \max_{(i)} \{(b_i-a_i)\} = \|b-a\| , \tag{4.5}$$

and the *midpoint* of X is $m(X) = \frac{1}{2}(a+b)$. The matrix norm corresponding to (4.1) for matrices $A = (a_{ij})$ is

$$\|A\| = \max_{(i)} \sum_{j=1}^{n} |a_{ij}| . \tag{4.6}$$

It follows from this and (4.4) that

$$\|A\| = |A[-e,e]| . \tag{4.7}$$

For a matrix $M = ([\alpha_{ij},\beta_{ij}])$ with interval components, one has

$$|M| = \max_{(i)} \sum_{j=1}^{n} |[\alpha_{ij},\beta_{ij}]| = \max_{A\in M} \{\|A\|\} = |M[-e,e]| . \tag{4.8}$$

In Theorem 3.2, suppose that $B \geq \|Y\|$, $\eta \geq \|y-w\|$, where $w = y - Y f(y)$, and

$$X_\rho = [y - \rho e, y + \rho e] = \bar{U}(y,\rho) . \tag{4.9}$$

The Krawczyk transformation of X is thus

$$K(X_\rho) = w + \rho\{I - YF'(X_\rho)\}[-e,e] . \tag{4.10}$$

Also, suppose that

$$\omega(\rho) \geq |Y^{-1} - F'(X_\rho)| . \tag{4.11}$$

Lemma 4.1. If $B\omega(\rho) < 1$, then $K(X_\rho) \subset X_\rho$ for

$$\rho \geq \frac{\eta}{1 - B\omega(\rho)} \quad . \tag{4.12}$$

Proof: As I,Y are real matrices, one may write

$$\{I-YF'(X)\} = Y\{Y^{-1}-F'(X)\} \quad . \tag{4.13}$$

For $v \in \rho\{I-YF'(X)\}[-e,e]$, $(w+v) \in K(X_\rho)$, and

$$\|y - (w+v)\| \leq \|y-w\| + \|v\| \leq \eta + B\rho\omega(\rho), \tag{4.14}$$

so that $\|y - (w+v)\| \leq \rho$ if (4.12) holds, and thus $(w+v) \in X_\rho$. QED.

An interval of the form $[-a,a]$ is said to be *symmetric*. As a linear transformation of a symmetric interval is symmetric, one has

$$\{I - YF'(X_\rho)\}[-e,e] = [-c,c], \tag{4.15}$$

and thus $K(X_\rho) = [w-\rho c, w+\rho c]$. The next step in the comparison of Theorems 3.1 and 3.2 will be to use the Lipschitz continuity of f' to obtain a scalar majorant function for $\omega(\rho)$. If f' is Lipschitz continuous on an interval X (with Lipschitz constant κ), then each component f'_{ij} of f' is also Lipschitz continuous on X, that is

$$|f'_{ij}(u) - f'_{ij}(v)| \leq \lambda_{ij}\|u-v\| \quad , \quad u,v \in X \quad . \tag{4.16}$$

Define

$$\lambda = \max_{(i)} \sum_{j=1}^{n} \lambda_{ij} \quad . \tag{4.17}$$

It follows that λ will be a Lipschitz constant for f' on X, so that one may assume $\kappa \leq \lambda$.

Lemma 4.2. If $y \in X$, then

$$|f'(y) - F'(X)| \leq \lambda|y-X|. \tag{4.18}$$

Proof: By (3.10), (4.4), and (4.16),

$$|f'_{ij}(y) - F'_{ij}(X)| \leq \lambda_{ij} \max_{x \in X} \{\|y-x\|\} = \lambda_{ij}|y-X|, \tag{4.19}$$

$i,j = 1,2,\ldots,n$. Inequality (4.18) now follows from (4.8), (4.16), and (4.17). QED.

The choice $Y = [f'(y)]^{-1}$ now gives a metric theorem which allows direct comparison of Theorems 3.1 and 3.2.

Theorem 4.1. If

$$h = B\lambda\eta \leq \frac{1}{4} \quad , \tag{4.20}$$

then $K(X_\rho) \subset X_\rho$ for ρ such that

$$\frac{1 - \sqrt{1-4h}}{2h}\eta \leq \rho \leq \frac{1 + \sqrt{1-4h}}{2h}\eta \tag{4.21}$$

and $X_\rho \subset X$.

Proof: As $y = m(X_\rho)$ is the midpoint of X_ρ, $|y-X_\rho| = \frac{1}{2} w(X_\rho) = \rho$, and one may take

$$\omega(\rho) = \lambda\rho \tag{4.22}$$

by (4.11) and (4.18). Thus, if $h \leq \frac{1}{4}$, then inequality (4.12) may be solved to give (4.21), and the conclusion follows from Lemma 4.1. QED.

In order to use Theorem 4.1 to compare the theorems of Kantorovich and Moore, it is natural to take $y = x^{(0)}$, $Y = Y_0$, where

$$Y_0 = [f'(x^{(0)})]^{-1}, \tag{4.23}$$

so that $w = x^{(1)}$, $B = B_0$, $\eta = \eta_0$. Thus, for

$$X^{(0)} = [x^{(0)} - 2\eta_0 e, x^{(0)} + 2\eta_0 e] = \Omega, \tag{4.24}$$

one has

$$K(X^{(0)}) = x^{(1)} + 2\eta_0\{I - Y_0 F'(X^{(0)})\}[-e,e]. \tag{4.25}$$

Corollary 4.1. Under the hypotheses of Theorem 3.1, if

$$h_0 \leq \frac{\kappa}{4\lambda}, \tag{4.26}$$

then $K(X^{(0)}) \subset X^{(0)}$.

Proof: This follows immediately from Theorem 4.1, as $h_0 = (\lambda/\kappa)h$. QED.

Remark 4.1. As (4.26) requires that $h_0 \leq \frac{1}{4}$ even if $\kappa = \lambda$, Corollary 4.1 provides a comparison of Theorem 3.1 with Theorem 3.2 which is unfavorable to the latter. Furthermore, this cannot be improved in general, as the following example shows. In R, take $f(x) = x^2 - \varepsilon^2$ for $0 \leq \varepsilon \leq 1$ and $x^{(0)} = 1$. This gives

$$x^{(1)} = \frac{1}{2}(1 + \varepsilon^2), \quad \eta_0 = \frac{1}{2}(1 - \varepsilon^2), \tag{4.27}$$

from which $X^{(0)} = [\varepsilon^2, 2 - \varepsilon^2]$. As $B_0 = \frac{1}{2}$ and $\kappa = \lambda = 2$, it follows that

$$h_0 = h = \frac{1}{2}(1 - \varepsilon^2), \tag{4.28}$$

and Theorem 3.1 guarantees the existence of the solution $x^* = \varepsilon$ of $f(x) = 0$ in $X^{(0)}$ for $0 \leq \varepsilon \leq 1$. On the other hand, direct computation with (4.25) yields

$$K(X^{(0)}) = [-\frac{1}{2} + \frac{5}{2}\varepsilon^2 - \varepsilon^4, \frac{3}{2} - \frac{3}{2}\varepsilon^2 + \varepsilon^4], \tag{4.29}$$

and it is easy to verify that $K(X^{(0)}) \subset X^{(0)}$ if and only if $\frac{1}{2} \leq \varepsilon^2 \leq 1$, that is, $0 \leq h_0 \leq \frac{1}{4}$.

A result more favorable to Moore's theorem may be obtained by making different choices of y, Y, and X than those above. If the hypotheses of Theorem 3.1 are satisfied, then the Newton sequence $\{x^{(k)}\}$ generated by (3.17) is well defined, as are the sequences of real numbers $\{\eta_k\}$, $\{B_k\}$, $\{h_k\}$ satisfying the relationships

$$
(4.30)\qquad \begin{cases} \eta_{k+1} = \dfrac{1}{2}\,\dfrac{h_k \eta_k}{1-h_k} \geq \|x^{(k+2)} - x^{(k+1)}\|, \\ B_{k+1} = \dfrac{B_k}{1-h_k} \geq \|[f'(x^{(k+1)})]^{-1}\|, \\ h_{k+1} = \dfrac{1}{2}\left(\dfrac{h_k}{1-h_k}\right)^2 = B_{k+1}\kappa\eta_{k+1}, \end{cases}
$$

$k = 0,1,2,\ldots$ [6; 15, pp. 135-138]. It is easy to verify that $\eta_k \leq 2^{-k}\eta_0$, and thus

$$
(4.31)\qquad X^{(k)} = [x^{(k)} - 2\eta_k e\,,\; x^{(k)} + 2\eta_k e] \subset X^{(0)}\,.
$$

Theorem 4.2. If the hypotheses of Theorem 3.1 hold with

$$
(4.32)\qquad h_0 \leq \frac{1}{2}\,,
$$

then there exists a positive integer k such that for $y = x^{(k)}$, $Y = Y_k = [f'(x^{(k)})]^{-1}$, one has $K(X^{(k)}) \subset X^{(k)}$.

Proof: If (4.32) holds, then the numbers h_k decrease rapidly with k. In fact, the recurrence relations (4.30) can be solved [3] to give

$$
(4.33)\qquad h_k = \frac{2\theta_0^{2^k}}{\left(1+\theta_0^{2^k}\right)^2}\,, \quad k = 0,1,2,\ldots\,,
$$

where

$$
(4.34)\qquad \theta_0 = \frac{1 - \sqrt{1-2h_0}}{1 + \sqrt{1-2h_0}}\,,
$$

and $\theta_0 < 1$ if (4.32) holds. Thus, a positive integer k will exist such that

$$
(4.35)\qquad h_k \leq \frac{\kappa}{4\lambda}
$$

and the conclusion will follow from Theorem 4.1, as $h = (\lambda/\kappa)h_k \leq \frac{1}{4}$. QED.

Remark 4.2. The condition (4.32) implies quadratic convergence of the Newton sequence $\{x^{(k)}\}$ to x^*; furthermore, x^* will be unique in $X^{(0)}$ and a simple zero of f in the sense that $[f'(x^*)]^{-1}$ will exist [16]. The case $h_0 = \frac{1}{2}$ is a borderline situation, which corresponds to linear convergence of the Newton sequence with ratio $\frac{1}{2}$ [6]. Consequently, if rapid convergence of the Newton sequence to the approximate solution y has been observed computationally, then it is likely that the value of h_0 corresponding to $x^{(0)} = y$ satisfies (4.26) immediately so that either Theorem 3.1 or 3.2 is applicable.

5. Precision and sensitivity to simple zeros. On the assumption that h_0 satisfies (4.26), it follows from Thereom 3.1 that for $y = x^{(0)}$,

$$\|y - x^*\| \leq \frac{1 - \sqrt{1-2h_0}}{h_0}\,\eta_0 = \rho_0 , \tag{5.1}$$

and, similarly, Theorem 4.1 gives, by (4.20),

$$\|y - x^*\| \leq \frac{1 - \sqrt{1-4(\lambda/\kappa)h_0}}{2(\lambda/\kappa)h_0}\,\eta_0 = \rho . \tag{5.2}$$

If $0 < h_0 \leq \kappa/4\lambda$, then it is evident that

$$\rho_0 < \rho , \tag{5.3}$$

so that the Kantorovich theorem is of greater precision than the metric version of Moore's theorem. However,

$$\lim_{h_0 \to 0} \frac{\rho_0}{\rho} = 1 , \tag{5.4}$$

so that the difference may be inconsequential for h_0 sufficiently small.

To compare sensitivity, suppose that x^* is a simple zero of f, and

$$B^* \geq \|[f'(x^*)]^{-1}\| . \tag{5.5}$$

Given Lipschitz constants κ,λ in a sufficiently large region Ω containing x^*, one may take

$$h_0 = \frac{1 - \frac{1}{2}B^*\kappa\|x^{(0)}-x^*\|}{(1-B^*\kappa\|x^{(0)}-x^*\|)^2}\,B^*\kappa\|x^{(0)}-x^*\| \tag{5.6}$$

in Theorem 3.1, provided that $\|x^{(0)}-x^*\| < 1/B^*\kappa$ [16]. From (5.6),

$$\|x^{(0)} - x^*\| \leq \frac{1}{B^*\kappa}\left(1 - \frac{\sqrt{1+2h_0}}{1+2h_0}\right) = \sigma(h_0) , \tag{5.7}$$

which may be used as a measure of sensitivity. From Theorem 3.1, x^* will be detected if

$$\|x^{(0)} - x^*\| \leq \sigma(\tfrac{1}{2}) , \tag{5.8}$$

that is, if $x^{(0)} \in \bar{U}(x^*,\sigma(\frac{1}{2}))$, while Corollary 4.1 requires that

$$\|x^{(0)} - x^*\| \leq \sigma\left(\frac{\kappa}{4\lambda}\right) . \tag{5.9}$$

Thus, as

$$\frac{\sigma(\frac{1}{4})}{\sigma(\frac{1}{2})} = \frac{2}{3}\left(\frac{3-\sqrt{6}}{2-\sqrt{2}}\right) = 0.6265\ldots , \tag{5.10}$$

the best radius of detection of x^* that can be guaranteed for the metric version of Moore's theorem is about 62.5% of the corresponding value for the Kantorovich theorem. The example of Remark 4.1 can also be used to show that this cannot be improved in general. As in Theorem 4.2, however, if $\|x^{(0)} - x^*\| < \sigma(\frac{1}{2})$, then $h_0 < \frac{1}{2}$, and there will exist a positive integer k such that

$$\|x^{(k)} - x^*\| \leq \sigma\left(\frac{\kappa}{4\lambda}\right) \tag{5.11}$$

for $x^{(k)}$ belonging to the Newton sequence $\{x^{(k)}\}$, and Moore's theorem with $y = x^{(k)}$, $Y = Y_k = [f'(x^{(k)})]^{-1}$, $X^{(k)} = [x^{(k)} - 2\eta_k e, x^{(k)} + 2\eta_k e] = X$ will detect x^*. The number of iterations required to obtain $\|x^{(k)} - x^*\| \leq \sigma(\frac{1}{4})$ is shown in Table 5.1 for various values of h_0.

h_0	k
0.41421	1
0.47648	2
0.49397	3
0.49848	4
0.49962	5
0.49990	6
0.49997	7
0.49999	8

Table 5.1.

Iterations Required to Ensure $h_k \leq \frac{1}{4}$.

6. Computational complexity. The computer program [9] for the implementation of the Kantorovich theorem has been adapted to apply Moore's theorem for the choices of y, Y, and X indicated for Corollary 4.1, and, as an additional option, for the choice

$$Y = [m(F'(X))]^{-1} \tag{6.1}$$

recommended by Moore and Jones [13]. This program provides an experimental as well as a theoretical basis for the comparison of the computational complexity of Theorem 3.1 with Theorem 3.2.

To make effective use of either theorem, software is needed for automatic differentiation [7] and implementation of interval computation for arithmetic operations and functions ordinarily encountered in FORTRAN expressions [17]. In addition, the program for the Kantorovich theorem requires software for interval matrix inversion [5; 11, pp. 32-39] as part of the painstaking calculations required to guarantee that upper bounds B_0, κ, η_0 are obtained for the quantities indicated in (3.1), (3.2), and (3.4) as results of inexact computations with machine numbers.

As the endpoints of intervals employed in actual calculations must be machine numbers, directed rounding is used after each operation to preserve the inclusion relationship. For this and other reasons [11], instead of the exact interval extension G of a continuous function g, a *computed extension* $\bar{G}$ is obtained, which has the property that $\bar{G}(X) \supset G(X)$ for all X. Thus, $|\bar{G}(X)| \geq |G(X)|$ and $\bar{G}(X) \subset X$ implies $G(X) \subset X$, so that rigorous conclusions can be drawn on the basis of interval calculations with computed extensions. In what follows, it will be convenient to identify a machine (or real) number z with the *degenerate interval* $z = [z,z]$.

The calculation of B_0, η_0 for the Kantorovich theorem are fairly straightforward applications of interval analysis. The Lipschitz constant κ, however, will be obtained from a bound for the second derivative

$$f''(x) = \left(\frac{\partial^2 f_i(x)}{\partial x_j \, \partial x_k} \right), \tag{6.2}$$

which will be called the *Hessian* of f. For a real bilinear operator $Q = (q_{ijk})$ in R_∞^n,

$$\|Q\| = \max_{\|x\|=1} \|Qx\| \leq \max_{(i)} \sum_{j=1}^{n} \sum_{k=1}^{n} |q_{ijk}| = \mu(Q), \tag{6.3}$$

with a similar expression for $|Q|$ if the elements of Q are intervals. Thus,

a machine number κ such that

$$\kappa \geq \mu(\bar{F}''(X)) = \max_{(i)} \sum_{j=1}^{n} \sum_{k=1}^{n} |\bar{F}''_{ijk}(X)|, \tag{6.4}$$

where $\bar{F}''$ is the computed extension of f'', will be a Lipschitz constant for f' on X, as

$$\kappa \geq \max_{x \in X} \|f''(x)\|. \tag{6.5}$$

The essential interval operations to implement the Kantorovich theorem will now be listed, it being assumed that $x^{(0)} = [x^{(0)}, x^{(0)}]$ is an exact machine vector:

K1. $\bar{F}(x^{(0)})$ is evaluated.

K2. The interval Jacobian $\bar{F}'(x^{(0)})$ is calculated.

K3. $\bar{Y}_0 \supset [F'(x^{(0)})]^{-1}$ is obtained by interval matrix inversion of $\bar{F}'(x^{(0)})$.

K4. $B_0 \geq |\bar{Y}_0| \geq \|[f'(x_0)]^{-1}\|$ is obtained by interval arithmetic, using (4.8).

K5. $\bar{W} = x^{(0)} - \bar{Y}_0 \bar{F}(x^{(0)})$ is computed using interval arithmetic, so that $x^{(1)} \in \bar{W}$ for the exact Newton point.

K6. $\eta_0 \geq |x^{(0)} - W| \geq \|x^{(1)} - x^{(0)}\|$ is obtained from (4.4) by interval arithmetic.

K7. $\bar{X} \supset [x^{(0)} - 2\eta_0 e, x^{(0)} + 2\eta_0 e]$ is constructed, using interval arithmetic.

K8. $\bar{F}'(\bar{X})$ is evaluated to obtain

K9. $\bar{F}''(\bar{X})$ by differentiation.

K10. $\kappa \geq \mu(\bar{F}''(\bar{X})) \geq \max_{x \in \bar{X}} \|f''(x)\|$ is obtained from (6.4) by interval arithmetic.

K11. $h_0 \geq |B_0 \kappa \eta_0|$ is calculated, using interval arithmetic.

After the machine number h_0 has been obtained in this way, it is checked versus the machine number $\frac{1}{2}$ to see if (3.5) holds to complete the automation of Theorem 3.1.

In the case of the Moore theorem, interval matrix inversion is avoided by evaluating $f'(x^{(0)})$ approximately as a real matrix, say in double precision, and then inverting the result carefully to obtain a real matrix Y which is the inverse of <u>some</u> matrix. (A failure of matrix inversion here or in K3 results in an exit from the program with an appropriate error indication.) The interval computations required for Moore's theorem with $y = x^{(0)}$ are:

M1. $\bar{F}(y)$ is evaluated.

M2. $w = y - Y\bar{F}(y)$ is computed using interval arithmetic; one has $w \in \bar{W}$.

M3. $\eta \geq |\bar{W}|$ is obtained from (4.4) by interval arithmetic.

M4. $\bar{X} \supset [y - 2\eta e,\ y + 2\eta e]$ is constructed by interval arithmetic.

M5. $\bar{F}'(\bar{X})$ is evaluated.

M6. $\bar{K}(\bar{X}) \supset \bar{W} + 2\eta\{I - Y\bar{F}'(\bar{X})\}[-e,e]$ is constructed by interval arithmetic.

These calculations result in the intervals $\bar{X} = [a,b]$, $\bar{K}(\bar{X}) = [c,d]$, where the components of the vectors a,b,c,d are all machine numbers. The verification of $\bar{K}(\bar{X}) \subset \bar{X}$ thus depends on checking the $2n$ inequalities

$$a_i \leq c_i, \quad d_i \leq b_i, \quad i = 1,2,\ldots,n, \tag{6.6}$$

between machine numbers.

Comparison of the lists of interval operations for the two theorems reveals that M1 = K1, M2 $\leq$ K5 (Y is a real matrix, so obtaining $Y\bar{F}'(y)$ generally requires fewer operations than for $\bar{Y}_0\bar{F}'(x^{(0)})$), M3 = K6, M4 = K7, M5 = K8. This commonality of subroutines made adaption of the original program to the new theorem very easy. This leaves K2, K3, K4, K10, K11 for implementation of Theorem 3.1 as against M6 and the inversion of a real matrix for automation of Theorem 3.2. In particular, K3 (interval matrix inversion) is tedious, and K9 (Hessian evaluation) requires $\frac{1}{2}n^2(n+1)$ differentiations and interval evaluations, while M6 is a simple interval matrix-vector multiplication.

It follows that the application of Theorem 3.2 is less complex by far than the use of Theorem 3.1. At least for good approximations $y = x^{(0)}$ to x^*, there is no significant difference in precision or sensitivity to offset this advantage of Moore's theorem.

A comment is in order on the choice (6.1) for Y. For $X = X_\rho$,

$$\left|m(F'(X_\rho)) - F'(X_\rho)\right| = \frac{1}{2}w(F'(X_\rho)), \tag{6.7}$$

and from (4.16) and (4.17),

$$w(F'(X_\rho)) \leq \lambda w(X_\rho) = 2\lambda\rho. \tag{6.8}$$

Thus, one may take $\omega(\rho) = \lambda\rho$ in Lemma 4.1, which gives Theorem 4.1 with

$$B \geq \|[m(F'(X_\rho))]^{-1}\|, \quad \eta \geq \|w-y\| = \|Yf(y)\|. \tag{6.9}$$

Here, however, ρ is chosen first, and (4.21) must hold if $h = B\lambda\eta \leq \frac{1}{4}$. Computationally, this method differs from the above in that M_3 and M_4 are eliminated, M5 follows the choice of X_ρ, $m(\bar{F}'(X_\rho))$ is then evaluated and inverted to obtain Y and then M1, M2, and M6 with $2\eta = \rho$ complete the computation. There is thus no essential difference in complexity.

7. A numerical example. An actual comparison of computational efficiency was obtained by applying the computer program [9], modified to include the implementation of Moore's theorem, to the quadratic system

$$x_i - \alpha x_i \sum_{j=1}^{9} a_{ij} x_j - 1 = 0 , \quad i = 1,2,\ldots,9, \tag{7.1}$$

with

$$a_{ij} = \frac{3}{4} \frac{t_i (1-t_j^2)^2 w_j}{t_i + t_j} , \tag{7.2}$$

where t_i, w_i, $i = 1,2,\ldots,9$, are respectively the nodes and weights of the Gaussian integration rule of order 17 on the interval $0 \le t \le 1$ [10, p. 288]. The system (7.1) was constructed as a discrete approximation to the nonlinear integral equation

$$x(s) = 1 + \frac{3\alpha}{4} s\, x(s) \int_0^1 \frac{(1-t^2)^2}{s+t} x(t)dt, \qquad 0 \le s \le 1 , \tag{7.3}$$

which is a case of the H-equation of Chandrasekhar [1, p. 105]. The value of α considered was $\alpha = 0.7$, and the initial approximation $y = x^{(0)} = e$ gave

$$\bar{X} = [0.3405052e, 1.6594949e]. \tag{7.4}$$

(Directed rounding is used in the conversion of intervals from binary to decimal; hence, the decimal interval $\bar{X}$ given by (7.4) contains the binary interval stored in the computer.)

The program for the Kantorovich theorem computed

$$h_0 = 0.700800 > \frac{1}{2} , \tag{7.5}$$

and thus failed to detect the existence of a solution $x^* = (x_1^*, x_2^*, \ldots, x_9^*)$ of (7.1) in $\bar{X}$. A total of 21.4652 UNIVAC 1110 time units were required, of which 4.7436 were expended for interval matrix inversion (K3 and K4), and 12.1394 were required for the evaluation of the Hessian (K9 and K10).

The program for the Moore theorem, on the other hand, required only a total of 5.4120 time units, and gave $\bar{K}(\bar{X}) \subset \bar{X}$, thus guaranteeing the existence of a solution $x^* \in \bar{K}(\bar{X})$. The components of $\bar{K}(\bar{X}) = [c,d]$ are given in Table 7.1.

In this simple example, the value of h_0 has not been overestimated badly, as the Hessian is constant, and all its nonzero elements have the same sign. For bilinear operators Q of this type, $\mu(Q) = \|Q\|$. Thus, the program based on Moore's theorem provides more information in this case, as well as showing the expected decrease in execution time. For systems with nonconstant Hessians, the advantage in speed of Theorem 3.2 should be even greater than the 4 to 1 advantage observed here. In addition, the flexibility of being able to use intervals other

i	c_i	d_i
1	1.0042228	1.0606792
2	1.0135268	1.1943671
3	1.0223478	1.3211143
4	1.0293528	1.4217681
5	1.0344997	1.4957230
6	1.0381216	1.5477668
7	1.0405689	1.5829316
8	1.0421079	1.6050443
9	1.0429109	1.6165838

Table 7.1. The Interval $\bar{K}(\bar{X}) = [c,d]$.

than balls and the componentwise error bounds furnished by intervals may be of significant advantage in practical computation.

The Author wishes to acknowledge the assistance of Julia H. Gray, S. T. Jones, and C. T. Kelley with this example, which arose in an investigation completely unrelated to the subject of this paper.

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In order to be useful, an approximate solution y of a nonlinear system of equations $f(x) = 0$ in R^n must be close to a solution x^* of the system. Two theorems which can be used computationally to establish the existence of x^* and obtain bounds for the error vector $y-x^*$ are the 1948 result of L.V. Kantorovich and the 1977 interval analytic theorem due to R.E. Moore. The two theorems are compared on the basis of sensitivity (ability to detect a solution x^* close to y), precision (ability to give sharp error bounds), and computational complexity (cost). A theoretical comparison shows that the Kantorovich theorem has at best

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Abstract (continued)

only a slight edge in sensitivity and precision, while Moore's theorem requires far less computation to apply, and thus provides the method of choice. This conclusion is supported by a numerical example, for which available UNIVAC 1108/1110 software is used to check the hypotheses of both theorems automatically, given y and f.